Approximating the Hurwitz Zeta Function

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Abstract

This project aims to implement a MATLAB function that approximates the Hurwitz zeta function $\zeta(s, a)$. This is necessary because the naive implementation fails for certain input near critical values for s and for a. Other series representations of the Hurwitz zeta function converge rapidly but do not handle complex values of s and/or a. We also consider existing forms for the Hurwitz zeta function, including one given by Bailey and Borwein, and evaluate their overall performance.

1 Introduction

The Hurwitz zeta function was introduced by Adolf Hurwitz in [7] as a natural generalization of the more famous Riemann zeta function, which itself is popularly known for its role in the Riemann zeta hypothesis. The Riemann zeta function itself is linked to a broad variety of applications, including finding numerical estimates for prime density, such as in the prime number theorem, as well as computing the Casimir effect in quantized fields [6], an intriguing quantum mechanical phenomenon that can be observed between two parallel, uncharged conducting plates. In addition, Barone Adesi et al [2] present an analytic continuation of the Hurwitz zeta function and provide an application to calculating the pair production rate of Dirac particles under certain conditions. Furthermore, the Hurwitz zeta function has been used to theoretically model the empirically observed Zipf-Mandelbrot law regarding text frequencies in random corpuses [10]. More abstractly, the Hurwitz zeta is related to the Bernoulli polynomials through a set of identities on rational values of the function. The Hurwitz zeta function can also be written as a series involving the gamma function, as the sum of Dirichlet L-functions [8], and for positive integer inputs, in terms of the polygamma function [1].

Accurately approximating the Hurwitz zeta function is thus significant due to its important applications in quantum mechanics and in other areas of mathematics. Coffey [3] provides various convergent, recursive expressions for the Hurwitz zeta function. Meanwhile, Bailey and Borwein [1] provide easily-computable series with rapid convergence for evaluating the incomplete Gamma function and the Lerch transcendent.

They cite and extend an efficient method found by Crandall [4] for computing the Hurwitz zeta function; for instance, the thirtieth partial sum of their series suffices to compute $\zeta\left(2, \frac{2}{3}\right)$ to 1000 digits of accuracy. Here, we present and evaluate various performance metrics regarding this and other series for the Hurwitz zeta function.

2 Definitions

In this section, we define the Hurwitz zeta function and some other relevant functions.

Definition. The **Hurwitz zeta function** $\zeta(s, a)$ is defined, for complex inputs s and a with $\mathrm{Re}(a) > 0$ and $\mathrm{Re}(s) > 1$, as follows:

$$\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}. \tag{1}$$

Note that $\zeta(s, 1) = \zeta(s)$.

The Hurwitz zeta function also has a meromorphic analytic continuation to complex s with $\mathrm{Re}(s) \leq 1$, defined for all complex $s \neq 1$ with a pole at $s = 1$.

$$\zeta(s, q) = \Gamma(1-s) \frac{1}{2\pi i} \int_C \frac{z^{s-1} e^{qz}}{1 - e^z} dz.$$

Definition. The **Lerch transcendent** $\Phi(s, a, z)$ is defined for complex inputs s,a,z as

$$\Phi(s, a, z) = \sum_{n=1}^{\infty} \frac{z^n}{(n+a)^s}.$$

The Lerch Transcendent further generalizes the Hurwitz zeta function.

Definition. 1. For a real number $s > 0$, the **gamma function** $\Gamma(s)$ is defined by the integral

$$\Gamma(s) = \int_0^{\infty} t^{s-1} e^{-t} dt.$$

When $s < 0$ and s not an integer, $\Gamma(s)$ is defined by the relation $s\Gamma(s) = \Gamma(s+1)$.

2. For real s, z, the **upper incomplete gamma function** $\Gamma(s, z)$ is defined by the integral

$$\Gamma(s, z) = \int_z^{\infty} t^{s-1} e^{-t} dt = \Gamma(s) - \int_0^z t^{s-1} e^{-t} dt.$$

Note that $\Gamma(s, 0) = \Gamma(s)$.

3 Alternative Representations of the Hurwitz zeta Function

In this section, we discuss some preexisting results regarding the Hurwitz zeta function and the gamma function. We first present a well-known integral adaptation of the Hurwitz zeta function that is valid for all s in the domain of the function.

Theorem 3.1. *For any complex numbers s and a such that $Re(s) > 1$ and $Re(a) > 0$,*

$$\zeta(s,a) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}e^{-at}}{1-e^{-t}} dt.$$

Unfortunately, when implemented directly into MATLAB, this expression provides an inferior approximation, compared to the series given in our definition, for default accuracy for around $|s| \approx 50$ at $a = 0.75$.

The following result analytically extends the Hurwitz zeta function to all complex $s \neq 1$:

Theorem 3.2. *For any $s \neq 1$,*

$$\zeta(s,a) = \frac{1}{s-1} \sum_{n=0}^{\infty} \frac{1}{n+1} \sum_{k=0}^{n} (-1)^k \binom{n}{k} (a+k)^{1-s}.$$

Unlike the series given in the definition of the Hurwitz zeta function, this expression for the function includes a nested summation. We would therefore expect more summands to be needed to compute $\zeta(s,a)$ to the same degree of accuracy, compared to the series given in the definition.

In [1, Theorem 7], Bailey and Borwein provide the following rapidly converging series for approximating the Hurwitz zeta function on real inputs a:

Theorem 3.3 (Bailey-Borwein [1])**.** *Let λ be a parameter with $0 < \lambda < 2\pi$. Define $\sigma(x)$ to be the sign function, so that $\sigma(0) = 0$ and $\sigma(x) = \frac{|x|}{x}$ otherwise. Then, for real a and complex s with $0 < a < 1$ and $Re(s) > 1$,*

$$\zeta(s,a) = \frac{\sqrt{\pi}\lambda^{\frac{s-1}{2}}}{(s-1)\Gamma\left(\frac{s}{2}\right)} + \frac{1}{2} \sum_{n=-\infty}^{\infty} \frac{1}{|n+a|^s} \left(\frac{\Gamma(\frac{s}{2}, \lambda(n+a)^2)}{\Gamma(\frac{s}{2})} + \sigma(n+a) \frac{\Gamma(\frac{s+1}{2}, \lambda(n+a)^2)}{\Gamma(\frac{s+1}{2})} \right)$$
$$+ \pi^{s-\frac{1}{2}} \sum_{m=1}^{\infty} \frac{1}{m^{1-s}} \left(\frac{\Gamma(\frac{1-s}{2}, \frac{m^2\pi^2}{\lambda})}{\Gamma(\frac{s}{2})} \cos(2\pi ma) + \frac{\Gamma(1-\frac{s}{2}, \frac{m^2\pi^2}{\lambda})}{\Gamma(\frac{s+1}{2})} \sin(2\pi ma) \right).$$

However, this expression,when implemented directly into MATLAB, diverges significantly from the series given in equation (1) for inputs s with $\text{Im}(s) \approx 100$ with $|\text{Re}(s)| \leq 5$. In contrast, the series given in (1) continues to produce accurate numeric results until around $\text{Im}(s) \approx 500$. .

We also present a representation of the Gamma function due to Weierstrass given in [5]:

Theorem 3.4 (Weierstrass)**.** *For any complex z not equal to a negative integer,*

$$\Gamma(z) = \frac{e^{-\gamma z}}{z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right)^{-1} e^{\frac{z}{n}}.$$

4 Issues with Direct Approximation

In using equation (1) directly to approximate the Hurwitz zeta function, as we might use to verify the accuracy of other approximations, some difficulties occur in some cases where the imaginary parts of s and a are relatively large.

When $n = 0$, the first term of the summation is equal to $\frac{1}{a^s}$. Set $a = e^{m+pi}$ and $s = \mathrm{Re}(s) + \mathrm{Im}(c)i = c + di$ for brevity, where $0 \le p < 2\pi$, and set, for instance, $0 < \mathrm{Re}(a) \le 1$. According to the rules of complex exponentiation, we have, for some suitable real argument k,

$$\begin{aligned} \left|\frac{1}{a^s}\right| &= \left|\frac{1}{(e^{m+pi})^{c+di}}\right| \\ &= \frac{1}{e^{mc-pd}} \\ &= \frac{e^{pd}}{|a|^c}. \end{aligned}$$

Thus, when $|a|^c \ll 1$ or $nd \gg 1$, $\frac{1}{a^s}$ may grow very large in magnitude.

If $\frac{\mathrm{Im}(a)}{\mathrm{Re}(a)} \gg 0$ and $d = \mathrm{Im}(s)$ is large, then the absolute value of the first term can explode; for instance, when $a = 0.5 + 100i, s = 0.5 + 100i$, we see that $\frac{1}{a^s} = \frac{e^{pd}}{|a|^c} \approx 0.1 \cdot e^{50\pi} \gg 10^{50}$. For such inputs, expansions starting at later n (such as $n = 30$) yield much better performance.

5 Analysis of Convergence

In this section, we evaluate the accuracy of partial sums of our series for the Hurwitz zeta function.

Theorem 5.1. *For any integer $N \gg |a|$, complex s, and real a with $Re(s) > 1$ and $a > 0$, we have*

$$\left|\sum_{n=N+1}^{\infty} \frac{1}{(n+a)^s}\right| < \frac{N^{1-Re(s)}}{Re(s) - 1}.$$

Proof. We first consider the convergence of our series in (1). Consider some large value $n > N \gg |a|$, and set $s = c + di$.

Recalling that a is a fixed constant, we have

$$
\begin{aligned}
\left|\sum_{n=N+1}^{\infty}\frac{1}{(n+a)^s}\right| &\leq \sum_{n=N+1}^{\infty}\frac{1}{|(n+a)^s|}\\
&= \sum_{n=N+1}^{\infty}\frac{1}{|n+a|^{\mathrm{Re}(s)}}\\
&\leq \sum_{n=N+1}^{\infty} n^{-\mathrm{Re}(s)}\\
&< \int_N^{\infty} t^{-\mathrm{Re}(s)}dt = \frac{N^{1-\mathrm{Re}(s)}}{\mathrm{Re}(s)-1}.
\end{aligned}
$$

□

Thus, we see that achieving k digits of precision using equation (1) requires $\Omega(10^{\frac{k}{\mathrm{Re}(s)-1}})$ terms of the summation, assuming perfect computation of each term, for some fixed s. This may not be feasible when $\mathrm{Re}(s) \approx 1$.

In preparation for our next result, we first roughly estimate the upper incomplete gamma function $\Gamma(s, z)$ for fixed real s and variable z for large values of z.

Lemma 5.2. *For $z > 2s$ and s real, we have*

$$\Gamma(s, z) < e^{(s-1)\ln z - z + 1}.$$

Proof. By the definition of the incomplete gamma function,

$$
\begin{aligned}
\Gamma(s, z) &= \int_z^{\infty} t^{s-1}e^{-t}dt\\
&< \sum_{i=z}^{\infty} i^{s-1}e^{-i} < \frac{z^{s-1}}{e^z(1-\frac{e^{s/z}}{e})} < e \cdot e^{(s-1)\ln z - z}
\end{aligned}
$$

as desired. □

We now prove a result regarding the convergence of individual terms in Theorem 3.3 for real s and a.

Theorem 5.3. *For real s and a with $s > 1$ and $a > 0$, and an integer n so that $|n + a| \geq \frac{s}{2}$ and $|n + a| \geq 10$,*

$$\Gamma\left(\frac{s}{2}, \pi(n+a)^2\right) < 10^{-(n+a)^2}.$$

Proof. We see by the lemma that

$$\begin{aligned}
\Gamma\left(\frac{s}{2}, \pi(n+a)^2\right) &< e^{(\frac{s}{2}-1)\ln \pi(n+a)^2 - \pi(n+a)^2+1} \\
&< e^{\frac{s}{2}\ln \pi(n+a)^2 - \pi(n+a)^2} \\
&\le e^{|n+a|\ln \pi(n+a)^2 - \pi(n+a)^2} \\
&< 10^{-(n+a)^2},
\end{aligned}$$

where the last equation holds as

$$(n+a)(\pi - \ln 10) > \ln \pi(n+a)^2$$

for all $(n+a) \ge 10$.

$\square$

Setting $\lambda = \pi$ (as recommended in [1]), we see that

$$\frac{1}{2}\sum_{|n|\ge N} \frac{1}{|n+a|^s}\left(\frac{\Gamma(\frac{s}{2}, \pi(n+a)^2)}{\Gamma(\frac{s}{2})} + \sigma(n+a)\frac{\Gamma(\frac{s+1}{2}, \pi(n+a)^2)}{\Gamma(\frac{s+1}{2})}\right) < \sum_{n=N}^{\infty} \frac{2}{\Gamma(\frac{s}{2})|n+a|^s}\left(10^{-(n+a)^2}\right),$$

which decreases faster than exponentially in N. A similar result holds for the second summation, due to the bounded trigonometric coefficients within the summands. Thus, assuming perfect accuracy of individual terms, the N-th partial sum of the summation yields $\Omega(N^2)$ digits of accuracy, a marked improvement over the simpler harmonic series. Indeed, [1] notes that summing the first 30 terms with $\lambda = \pi$ yields 1000 digits of accuracy for $\zeta(4, 2/3)$ or $\zeta(2, 2/3)$.

Thus far, our demonstrations of rapid convergence apply only to real arguments of s and/or a, and only provide an upper bound. It would be interesting to generalize our bounds to complex values for both s and a.

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